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Facility for Local Postprocessing, Visualization, and Animation of Remotely Simulated Very Large Temporal Datasets.

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This DURIP equipment Grant in support of ongoing AFOSR sponsored researach in the Division of Applied Mathematics at Brown University primary purpose of the equipment is to enhanced computationally intensive research in high-order numerical methods and high-performance computing currently supported under AFOSR Grant F49620-99-1-0077, High Order Methods for the Numerical Simulation of High Speed Flows. These efforts focused on the analysis and application of novel high-order schemes, designed specifically with contemporary parallel high performance computer arrchitectures in mind, for the solution of wave dominated transient problems in three dimensional complex geometries.

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Final Technical Report

Title: Facility for Local Postprocessing, Visualization, and Animation of Remotely Simulated Very Large Temporal Datasets.

Grant No: AFOSR F49620-00-01-0211

Grant Period: 04/01/2000 - 03/31/2001, 3 months no-cost extension to 06/31/2001.

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Technical Objectives

Grant # F49620-00-1-0211, entitled *Facility for Local Postprocessing, Visualization and Animation of Remotely Simulated Very Large Temporal Datasets* was a DURIP equipment Grant in support of ongoing AFOSR sponsored research in the Division of Applied Mathematics at Brown University. The primary purpose of the equipment is to enhance computationally intensive research in high-order numerical methods and high-performance computing currently supported under AFOSR Grant AFOSR F49620-99-1-0077, *High Order Methods for the Numerical Simulation of High Speed Flows* (P.I. - Gottlieb, Co-PI's - W.S. Don, J.S. Hesthaven, C.W. Shu; annual funding level, $180K) and by AFOSR/DARPA (on subcontract to HyperComp Inc.), *Advancing the Frontiers of Broad Band CEM for Modeling Full-Scale Treated Targets* (PI - D. Gottlieb; Co-PI - J.S. Hesthaven; Annual funding level, $200K). These efforts focuse on the analysis and application of novel high-order schemes, designed specifically with contemporary parallel high-performance computer architectures in mind, for the solution of wave dominated transient problems in three-dimensional complex geometries.

This work entails both fundamental and applied research in high-order approximation methods (e.g., essentially non-oscillatory (ENO/WENO) schemes, spectral methods, spectral element methods, and discontinuous Galerkin methods) for compressible flow simulations, combustion, electromagnetic scattering and penetration, and active flow control for flameholders as well as fundamental and applied work in algorithms for high-performance parallel computers.

Typical applications include three-dimensional modeling of jet-engine flameholders and shock enhanced supersonic combustion and mixing. Problems in electromagnetics include broad-band scattering by heterogeneous bodies and modeling of optical devices.

The establishment of the proposed facility paves the way for the ability to transfer, manipulate, and visualize very large temporal datasets resulting from the simulation of two- and three-dimensional transient phenomena in general complex geometries as those currently considered as part of the AFOSR sponsored research. With the resources available prior to the DURIP award, such large scale manipulations were not possible, hence essentially prohibiting the transfer of existing computational models to DOD HPC platforms due to an inability to effectively handle the very large datasets.

The facility, made possible by this grant, was designed to eliminate this bottleneck and facilitate a vastly extended use of DOD HPC resources to solved very large scale unsteady problems using high-order methods as part of AFOSR supported research and educational efforts. As we shall describe shortly, this has already been demonstrated and is certain to be invaluable for future efforts.

Equipment Purchased

A list of purchased equipment and approximate expense is given below.

Qty.	Item.	total
2	Compaq ES40 (4 750 MHz Alpha processors, 8GB RAM)	146,000
2	Myrinet Interface and Cable for ES40	2,690
4	SUN Blade 1000 (2 750 MHz Sparc III processors, 2GB RAM)	80,000
4	Fiber Channel Interface for SUN Blade	4,980
5	SUN Ultra 10 (1 450 MHz Sparc II processors, 1GB RAM)	12,915
5	Dell PC with 19" screen (1 1.4 GHz Pentium IV processors, 1GB RAM)	19,500
1	Xyratex RAID Array w/ powersupply and FiberChannel Interface	13,235
12	Xyratex 73.4 GB	13,560
2	Fiber Channel Cable	170
1	Brocade Fiber Channel Switch	15,887
12	Brocade Fiber Channel Cobber Gigabit Interconnect	1,478
4	Brocade Fiber Channel Fiber Gigabit Interconnect	1,254
1	Brocade Fiber Channel Switch Rack	235
2	SANergy Interface to Compaq ES40	6,200
4	SANergy Interface to SUN Blade 1000	12,400
2	SANergy Professional Installation	3,000
1	Exabyte X200 Archival Tape Library	38,615
100	DLT 225m Tapes	7,925
1	Tivoli/IBM Archival Software	10,000
2	Panasonic DVD-RAM for PC	1,090
2	PCI Ultra SCSI Cards	176
1	HP8500DN Large format color printer	7,500
2	HP4100SHE Laser Printers	2,300
	Total	401,110

The original proposal called for an entirely SUN based system. However, SUN was unable to offer a competitive server solution within a reasonable timeframe. The server plays a central role in the system for data-management and processing, price/performance of these was considered the main priority, hence the choice of the Compaq SE40 solution. As the main role of these machines are for dataprocessing and manipulation rather than graphics the less favorable graphics preformance of the Compaq solution poses no problem as the SUN and highend PC's all have excellent graphics performance.

The originally approved award was on $369,000 with an additional $30,000 from costsharing by Brown University, totalling $399,000. The remaining $2,110 was absorbed by Brown University.

Overview of Facility

The purpose of the facility is to support ongoing research and educational efforts centered around the development and application of novel high-order schemes. exemplified by spectral methods, spectral element methods on polymorphic domains, discontinuous Galerkin method and essentially non-oscillatory (ENO/WENO) schemes. Applications include the accurate simulation of transient phenomena in fluid and gas flows, combustion problems, electromagnetics and acoustics. The efforts also have very significant components of fundamental and applied algorithmic work for contemporary high-performance parallel computers.

The problems being considered in these efforts are characterized by a significant seperation of scales in time and space, eigther due to the dynamics of the problems as in supersonic gas-dynamics and combustion or as a consequence of the geometry of the problems as exemplified by broad-band electromagnetic or acoustic scattering by large heterogeneous bodies. In most cases the use of high-order methods is a necessity to obtain any reliable computational results for such problems.

All of these problems are, however, also characterized by a very significant temporal component in combination with a truly three-dimensional character, which necessitates the use of remote DOD HPC sites due to the computational complexity of a problem of realistic complexity

The facility enables a much needed expansion in the use of remote DOD HPC resources for the simulation of two- and three-dimensional transient phenomena in general complex geometries by significantly enhancing the ability to transfer as well as pre/post-process, visualize and animate very large temporal datasets.

The central components of the facility are the two Compaq ES40 servers, each with 4 750 MHz Alpha processors and 8GB of RAM. These servers provide the main source of computing power and ensure the ability to handle multiple instances of large datasets for processing, feature extraction etc.

Closely connected to these two servers are 4 SUN Ultra III based highend workstations, each with 2 750 MHz Sparc III processors, 2GB of RAM and highend graphics capabilities. These machines are used by senior researchers (faculty and postdocs) with extraordinary needs in terms of computing resources.

To support the ability to handle large datasets, a 840GB RAID accelerated discarray has been purchased. This, the 2 Compaq servers and the 4 SUN Ultra III workstations are all linked together in a dedicated very broadband storage network (SAN) based on Fiber Channel links. This ensures a very high data transfer rate between servers, discs and workstations for efficient data manipulation and visualization. The workload is split in such a way that the workstations perform the graphics rendering while compute intensive pre- and postprocessing is done by the servers. The SAN is also connected to the Brown IBM SP to serve as an testing platform as well as to the vBNS to ensure fast and reliable transferral of data to and from DOD HPC sites.

Initial trials with the graphics package Ensigth Gold suggested that this would serve as a common platform for visualization. However, given the different tasks to be performed we have chosen to use Tecplot as the main visualization tool. With its recent support of OpenGL this is found to give very good performance, a high degree of user friendliness as well as the flexibility needed on a platform serving educational as well as research goals.

A second ring of computing hardware consists of 5 highend Linux based PC's, equipped with 1.4 GHz Pentium IV processors, 1GB RAM, and highend graphics cards, as well as 5 SUN Ultra 10, Sparc II based workstations, each with 1GB RAM. These 10 machines serve the students, visitors, and faculty involved in the sponsored research. They are all connected to the facility by 100Mb Ethernet. Furthermore, as the need arises for particular individuals, access to faster and more closely connected hardware as described above will be granted.

The large disc array is configured with a large temporary space which it is the users respondsibility to backup. Regular backup is only offered on 200GB of the disc. To enable this, increased capasity of the archival tape libraries has been implemented with a dedicated archival system with a native capasity of up to 11TB. Furthermore, 2 DVD-RAM systems has been purchased to support used guided data transferral and storage as well as for storage of animations etc.

For offline data analysis, a large format high quality color laser printer has been purchased as well as two shared laser printers.

The central parts of the facility, i.e., the two Compaq servers, the 4 Sparc III workstations, the SAN

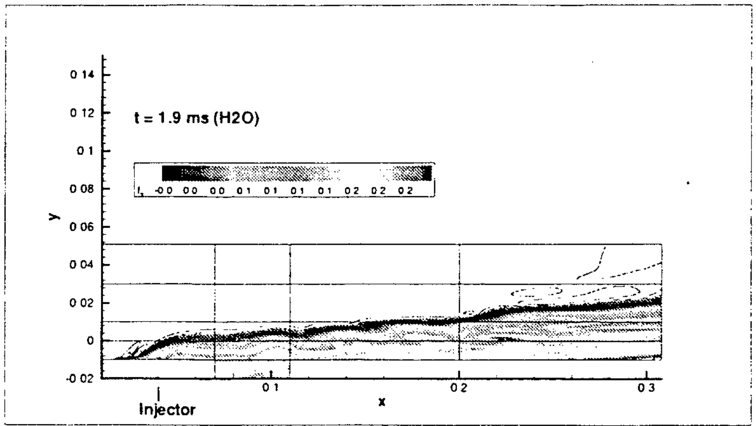

Figure 1: Two-dimensional computation of recessed cavity flameholder flow at a Reynolds number of $3.9 * 10^7$ (based on the free stream flow and a unit length) and a Mach number of 1.91. Shown is a snapshot of the water fraction. The model is the full compressible Navier-Stokes equations, coupled with a single reversible reaction to model the combustion of hydrogen in an oxygen/nitrogen atmosphere.

network and the large discarray, are logically seperated from the common network in the Division and access is granted only to students, visitors, and faculty directly involved in AFOSR sponsored research and educational efforts.

The acquisitions establishe a state-of-the-art post-processing and visualization facility for the senior investigators and students involved in the current AFOSR sponsored efforts. Moreover, it establishes a powerful computational platform for research-related education in areas of research relevant to the missions of DOD and will, due to the emphasis in the design of the facility on flexibility, expandability, and connectivity to existing resources, have an extended useful lifetime.

Impact on Applications

In the following we shall very briefly review some applications already taking advantage of the new facility which, in some cases, represent an enabling technology. These examples are not meant to be exhaustive but rather provide illustrations of current AFOSR sponsored efforts benefitting from the facility.

The applications are all characterised by inherent time-dependence, moderate to very high geometric complexity and/or the apparence of strong shock and near singular solutions.

While we have developed and tested various computational schemes over the last years, the lack of powerful local resources for the very demanding transfer, post-processing, and visualization of the large amounts of data resulting from these computations has essentially made it impossible to attempt the computation of realistic scenarios using DOD HPC resources.

The increased local bandwidth, the significant local storage, and the enhanced local computing power provided by the dedicated facility has been central to avoid that the data analysis be the limiting factor in the modeling of these types of problems. The reliable high-speed connections to DOD HPC through vBNS permits the transferral of large datasets to and from the sites and the local proposed facility facilitates the very significant task of manipulating, visualizing and post-processing the multiple instance datasets for realistic three-dimensional simulation.

Problems in Supersonic Mixing and Combustion

Ongoing work on high-order modeling of supersonic mixing and combustion has benefitted significantly from the facility. The main difficulty associated with the accurate modeling of the supersonic mixing and

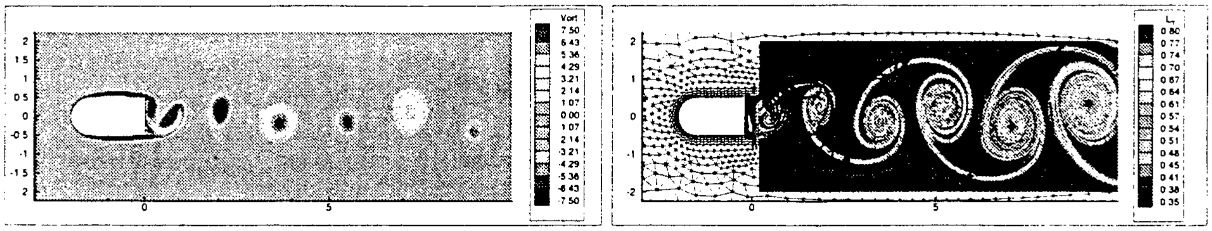

Figure 2: Shown is the result of the computation where Re = 10000, M = 0.3, using 6th order elements and a viscous gridding. The left illustrates the vorticity, clearly showing the von Karman street, while the right illustrates the identification of the structures computed using off-line particle tracking.

combustion is the extended range of scales that co-exist in the simulations which also are highly temporal in nature. This imposes the need for very high resolution in the simulations, typically exceeding 1024^2 spectral modes in two-dimensions and at least 512^3 modes for the fully three-dimensional problem. The temporal nature of the phenomena requires a multiple frame analysis to recover information about diffusion rates, the effects of chemical reactions etc.

As an example of a current effort we consider the accurate and detailed modeling of recessed cavity flameholders, typically operating in the supersonic flow-regime. Recessed cavity flameholders provide a high temperature, low speed recirculation zone that can effectively contain the production of radicals during chemical reactions and cavity flameholders are, therefore, being considered as an essential component for scram-jet propulsion systems with the advantages being their simplicity and their low total pressure losses for steady state flows.

To model the flameholders under realistic flow-conditions, e.g., at Mach numbers ranging from almost 0 to well above 2.5 and a Reynolds number exceeding 10^5, very high resolution and long time integration studies is required. It is exactly for this kind of problems that the facility has been designed, providing a front-end and post-processing facility to large scale parallel computations.

In Fig. 1 we illustrate the results of a recent computation, run in the supersonic regime with a simple model for the burning of hydrogen in a oxygen/nitrogen atmosphere. While these results are obtained using a spectral multidomain code, a parallel effort involves the solution of the same problem using high-order WENO methods.

We are using experimental data from WPAFB to verify and improve the computational effort. These experiments clearly illustrate the highly temporal and three-dimensional nature of the very complex phenomena and it is only through this kind of mutual interaction between computational modeling and detailed experimental data that the details of the flow scenarios can be understood.

Other related efforts, benefitting directly from the purchased equipment, include high-order modeling of Rayleigh-Taylor and Ritchmyer-Meshkov instabilities and the associated mixing. These efforts are again guided by solutions obtained with different schemes as well as by comparison with experimental results.

Problems in Flameholder Dynamics and Active Control

Another ongoing effort, directly and immediately benefitting from the facility, involves the modeling of bluff body flameholders with the aim of formulating active control schemes to enhance mixing. The typical scenario is characterized by a bluff body sitting within a narrow channel. The bluff body gives rice to the shedding of vortices, hence causing the flow to be periodic in nature — at least for low Reynolds numbers.

The computational model involves a high-order unstructured grid method, suitable for modeling fully compressible viscous gas-dynamics. The unstructured grid enables the accurate representation of the geometry, which can be rather complex with inlet-pipes etc for control of the flow, while the high-order accuracy ensures an accurate and reliable solution. The implementation is fully parallel and executes well on distributed computing platforms.

The computations serve as a virtual experiment through which one can gain understanding of the flow pattern and develop a simple, yet efficient active control loop to enhance the mixing by breaking up the structures formed rear of the flameholder.

In Fig. 2 we show the result of the computation with Re = 10000, $M = 0.3$, using 6th order elements and a viscous gridding. One clearly observes the von Karman vortex street rear of the bluff body. Figure 2 also shows how the use of results from dynamical systems theory allows one to clearly identify the structures. This is done in a post-processing phase, utilizing a large number of time-slices to track particles both forward and backward in time to identify the manifolds associated with the flow. The central idea is that one who controls the structures, controls the mixing. What is also shown is the structures, computed using massless tracers, and a few particle paths for finite mass particles, modeling finite size fuel drops in the flow.

This effort is ongoing and will continue to benefit significantly from the facility. The use of large datasets in which to track particles and many very long time computations to understand the flowpattern would not have been possible without the equipment. With this, we hope to develop efficient active flow control techniques and demonstrate their application to two- and three-dimensional flows.

Problems in Computational Electromagnetics and Acoustics

The development of new technologies such as ultra short pulse radars and integrated optics introduces an increased need for the accurate and efficient modeling of electromagnetic problems under circumstances involving very broad band signals and often electrically large objects or collections thereof. The need for the full vectorial solution of the electromagnetic problem subjected to a general time-dependent excitation suggests the use of time-domain methods in which plane wave and short pulse excitation in handled equally by directly solving the full vectorial Maxwell equations.

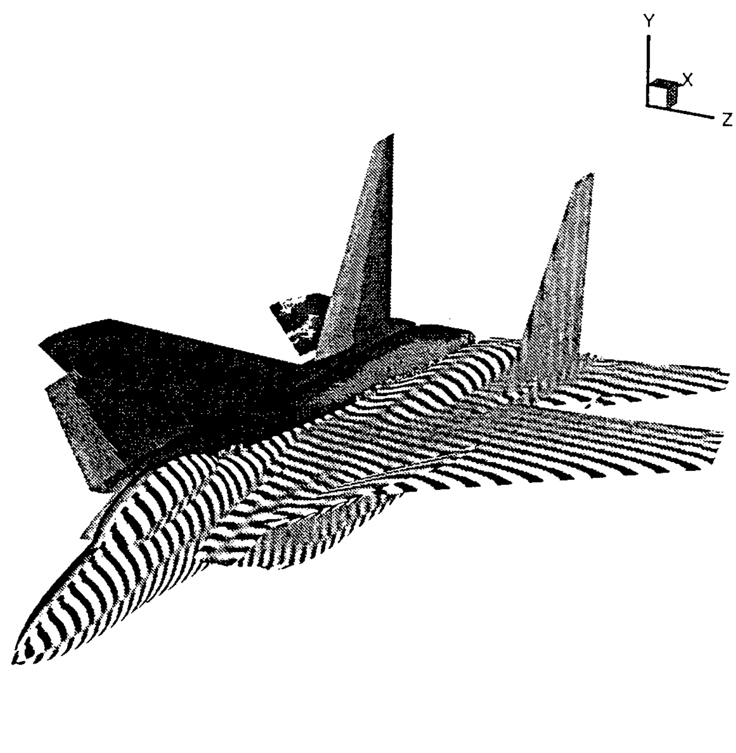

Figure 3: Nose to tail component of the reflected magnetic field from an incident plane wave.

To address such problems we have developed, over the past few years, a high-order/spectral time-domain solution methods for Maxwell's equation with the discretization of the computational domain being fully unstructured and body conforming. One of the novel aspects of this effort is the representation of the approximate solutions using truly multi-variate Lagrange interpolation polynomials much in the spirit of classical spectral collocation methods. Maxwell's equations are solved in a discontinuous element formulation, ensure a highly parallel scheme well suited for large scale distributed computing.

As an illustration of the ability of the proposed framework to address problems of realistic complexity, we show in Fig. 3 an example of electromagnetic plane wave scattering from a combat fighter plane. The finite element grid contains 123.000 elements for this case.

The scheme has been implemented on the local IBM SP as well as on the NAVO IBM SP for large scale computations. Recently, full three-dimensional computational modeling of 3.4 GHz scattering from a full aircraft configuration has been completed using this code on the NAVO IBM SP and up to 512 processors. The computations are done at 6th order accuracy, yielding an excess of 10^8 degrees of freedom. Each snap shot of the fields exceeds 1GB of data.

These computations and data manipulations would not have been possible without the facility which will be instrumental in the continuation of this effort.

Student Training

This is a one-year equipment grant which primarily addresses infrastructure improvements for scientific computing in the Division of Applied Mathematics at Brown and as such does not support individual researchers. However, the group involved in these activities currently consists of 3 faculty members, approximately 5 longterm visitors and postdoctoral researchers as well as an average of 10 graduate students. For most of these individuals, the facility will continue to enhance the ability to conduct research central to DOD missions.

Furthermore, with its state-of-the-art post-processing and visualization capability, the facility serves as an ideal platform for research-related education in a number of HPC related areas as well as in computational science, numerical analysis etc. Moreover, the vastly improved network infrastructure and connectivity to DOD HPC sites ensures reliable access to DOD facilities, hence allowing the students to exploit and take advantage of these facilities as a natural ingredient of their research efforts.